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Third and Fourth Order Accurate Schemes for Hyperbolic Equations of Conservation Law Form*

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Abstract. It is shown that for quasi-linear hyperbolic systems of the conservation form $W_t = -F_x = -AW_x$, it is possible to build up relatively simple finite-difference numerical schemes accurate to 3rd and 4th order provided that the matrix A satisfies commutativity relations with its partial-derivative-matrices. These schemes generalize the Lax-Wendroff 2nd order scheme, and are written down explicitly. As found by Strang [8] odd order schemes are linearly unstable, unless modified by adding a term containing the next higher space derivative or, alternatively, by rewriting the zeroth term as an average of the correct order. Thus stabilized, the schemes, both odd and even, can be made to meet the C.F.L. (Courant-Friedrichs-Lewy) criterion of the Courant-number being less or equal to unity. Numerical calculations were made with a 3rd order and a 4th order scheme for scalar equations with continuous and discontinuous solutions. The results are compared with analytic solutions and the predicted improvement is verified.

The computation reported on here was carried out on the CDC-3400 computer at the Tel Aviv University computation center.

1. Introduction. When dealing with one-dimensional problems in continuum mechanics, and, in particular, hydrodynamics, it is often necessary to solve nonlinear hyperbolic systems of the form

$$W_t + F_x = 0, \tag{1}$$

where $(\ )_t$ and $(\ )_x$ denote, respectively, partial differentiation with respect to the time and space coordinates. W is a vector whose components are the unknown functions and F is a vector whose components are dependent functionally on the components of W only. We consider the quasi-linear case where $F_x = AW_x$, A being a matrix whose components depend on the unknown functions only, and not on their derivatives. Since Eq. (1) is assumed to be hyperbolic, the eigenvalues of A are all real.

Systems of the form of Eq. (1) are called "Conservation Law Form" systems. Various numerical schemes for their solution have been developed, see [1], [2], [3], [4], [5], starting with Lax and Wendroff [1].

Keeping in mind that, ultimately, the main interest will focus on multidimensional systems, it is obviously important to develop numerical schemes whose order of accuracy is higher than one. A widely used 2nd order accuracy scheme is the one due to Lax and Wendroff [1]. Their finite-difference approximation is written thus:

$$W_j^{n+1} = W_j^n - \frac{\lambda}{2}(F_{j+1}^n - F_{j-1}^n) + \frac{\lambda^2}{2}[A_{j+1/2}^n(F_{j+1}^n - F_j^n) - A_{j-1/2}^n(F_j^n - F_{j-1}^n)] \tag{2}$$

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where

$$W_j^n = W(x_j, t_n), \qquad (j = 1, 2, \cdots, J = j_{\max}), (n = 0, 1, 2, \cdots),$$
$$\lambda = \Delta t/\Delta x.$$

If the problem contains discontinuities (such as shocks which may develop even if the initial conditions are smooth; see [6]), the system may be handled either by adding a nonlinear artificial viscosity term [1] or by iterative methods [4]. A stability criterion determines Δt_n for the predetermined and fixed Δx.

With a view towards multidimensional computations, it is of interest to consider 3rd order accuracy schemes for nonlinear hyperbolic equations of the type (1) where, for the present, we shall consider the scalar case, i.e., a simple conservation-form equation. A first attempt in this direction is due to Burstein [7] who developed a three-step approach in analogy to Richtmyer's two-step method [3] which approximates the Lax-Wendroff 2nd order scheme. We shall use the basic ideas of Lax and Wendroff [1] for estimating truncation errors in order to construct a third order scheme.

2. **Derivation of the Method.** The Lax-Wendroff (L-W) method is based on the fact that from the equation $W_t + F_x = 0$ one obtains

$$W_{tt} = (AF_x)_x. \tag{3}$$

This allows the construction of a 2nd order scheme by developing $W(x, t + \Delta t)$ in a Taylor series which, to order $(\Delta t)^2$, is given by

$$W(x, t + \Delta t) = W(x, t) + (\Delta t) W_t + \frac{(\Delta t)^2}{2!} W_{tt} + O(\Delta t^3)$$

and the time derivatives are replaced by space derivatives through the use of Eqs. (1) and (3). This provides a finite-difference scheme, where W is advanced in time by using only spatial differences.

Our first task is to construct a formula similar to Eq. (3) for higher order time derivatives. We make the following claim:

If the matrix A of the hyperbolic system (1) is commutative with its partial-derivative-matrices, then

$$\frac{\partial^n W}{\partial t^n} = (-1)^n \frac{\partial^{n-1}}{\partial x^{n-1}} (A^{n-1} F_x) \tag{4}$$

for every natural number n.

The proof proceeds as follows:

$$W_{tt} = (AF_x)_x = A_x F_x + AF_{xx}; \tag{5}$$

on the other hand,

$$W_{tt} = (-AW_x)_t = -A_t W_x - AW_{xt} = -A_t W_x + AF_{xx}. \tag{6}$$

Comparing (5) and (6), we obtain

$$A_t W_x = -A_x F_x = -A_x A W_x. \tag{7}$$

With these preliminaries and with our assertion (4), known to be true for $n = 1$ and 2 (even without the commutativity condition), we now consider the case $n = 3$:

(8) $W_{ttt} = [(AF_x)_x]_t = [(AF_x)_t]_x = [A_tF_x + AF_{xt}]_x = [A_tAW_x + A(-AF_x)_x]_x$.

Now substitute the commutativity restriction $A_tA = AA_t$ into (8) to get

$$W_{ttt} = [AA_tW_x - A(A_xF_x + AF_{xx})]_x.$$

Using (7), we obtain (using $A_xA = AA_x$):

$$\begin{aligned} W_{ttt} &= [A(-A_xF_x) - AA_xF_x - A^2F_{xx}]_x = [-2AA_xF_x - A^2F_{xx}]_x \\ &= -[(A^2)_xF_x + A^2F_{xx}]_x = -(A^2F_x)_{xx}. \end{aligned} \tag{9}$$

We have thus verified our claim (Eq. (4)) for the case $n = 3$. It is easy to show by induction that Eq. (4) is valid for all n.

With the aid of this result, we can construct a finite-difference scheme to any desired truncation error by writing the required Taylor series:

$$W(x, t + \Delta t) = W(x, t) + \sum_{k=1}^{m} (-)^k \frac{(\Delta t)^k}{k!} \frac{\partial^{k-1}}{\partial x^{k-1}} (A^{k-1}F_x) + O[(\Delta t)^{m+1}]. \tag{10}$$

One has only to take care to represent the various derivatives by a finite-difference expression which has the proper accuracy so that the overall scheme retains the desired truncation error. It should be noted that by the Cayley-Hamilton Theorem it is possible to express A^k ($k \geqq r$) in terms of $A, A^2, \cdots, A^{r-1}$, where A is of order $r \times r$.

It is interesting to note that the equations describing the fluid dynamic behavior of polytropic products of detonation with $\gamma = 3$ satisfy the commutativity restriction. For this situation, the system is described by

$$W = \begin{bmatrix} c \\ u \end{bmatrix}, \qquad F = \begin{bmatrix} uc \\ \frac{1}{2}u^2 + \frac{1}{2}c^2 \end{bmatrix}, \qquad A = \begin{bmatrix} u & c \\ c & u \end{bmatrix},$$

where c and u are the speed of sound and particle velocity, respectively, and γ is the polytropic constant. This system, where an equation of state of the form $p \sim \rho^\gamma$ is assumed, cannot describe solutions with strong shocks but can give very good approximations for expansion flows and flows with weak shocks [9], [10].

3. A Third Order Finite-Difference Scheme. We shall consider now the case of a system obeying the restriction on A

$$W_t = F_x = A(W)W_x, \tag{11}$$

with the initial condition

$$W(x, 0) = \Phi(x). \tag{12}$$

In order for all the terms in the finite-difference representation to be of at least of third order, it is necessary to improve the representation of the first derivative thus:

$$(V_x)_j^n = \frac{V_{j+1}^n - V_{j-1}^n}{2h} - \frac{V_{j+2}^n - 2V_{j+1}^n + 2V_{j-1}^n - V_{j-2}^n}{12h} + O(h^4). \tag{13}$$

It should be noted that for a third order accuracy scheme, one may still use $A^n_{j+1/2} = A[\frac{1}{2}(W^n_{j+1} + W^n_j)]$ or something equivalent; but for higher order schemes, it will be necessary to utilize a better interpolation.

We can now write down a finite-difference scheme of third order accuracy:

$$
\begin{aligned}
W_j^{n+1} = W_j^n &+ \lambda\left[\tfrac{1}{2}(F^n_{j+1} - F^n_{j-1}) - \frac{\delta}{12}(F^n_{j+2} - 2F^n_{j+1} + 2F^n_{j-1} - F^n_{j-2})\right] \\
&+ \frac{\lambda^2}{2}[A^n_{j+1/2}(F^n_{j+1} - F^n_j) - A^n_{j-1/2}(F^n_j - F^n_{j-1})] \\
&+ \epsilon\frac{\lambda^3}{6}[\tfrac{1}{2}(A^n_{j+1})^2(F^n_{j+2} - F^n_j) - (A^n_j)^2(F^n_{j+1} - F^n_{j-1}) \\
&\qquad + \tfrac{1}{2}(A^n_{j-1})^2(F^n_j - F^n_{j-2})]
\end{aligned}
\tag{14}
$$

with $\delta = \epsilon = 1$. If we set $\delta = \epsilon = 0$, we get back to the 2nd order accuracy scheme of Lax and Wendroff. Scheme (14) is unstable as it stands. In order to stabilize it, we have to add artificial viscosity terms. This requirement is typical in schemes of odd order of accuracy.

4. The Stabilizing Artificial Viscosity. We propose an artificial viscosity term of the form

$$
-\frac{\Omega}{24}h^4(\lambda^2A^2 + \nu\lambda^4A^4)W_{4x} \qquad (W_{4x} \equiv \partial^4W/\partial x^4).
\tag{15}
$$

The part of (15) which is proportional to $\lambda^2A^2W_{4x}$ results from expressing W_{tt} to a higher accuracy than $O(h^2)$. This improvement, if given in a conservation form, is written thus:

$$
\begin{aligned}
[(AF_x)_x]^n_j = &\frac{1}{h^2}[A^n_{j+1/2}(F^n_{j+1} - F^n_j) - A^n_{j-1/2}(F^n_j - F^n_{j-1})] \\
&- \frac{1}{12h^2}[A^n_{j+3/2}(F^n_{j+2} - F^n_{j+1}) - 3A^n_{j+1/2}(F^n_{j+1} - F^n_j) \\
&\qquad + 3A^n_{j-1/2}(F^n_j - F^n_{j-1}) - A^n_{j-3/2}(F^n_{j-1} - F^n_{j-2})].
\end{aligned}
\tag{16}
$$

It is the second term on the R.H.S. of (16) which gives rise to $\lambda^2A^2W_{4x}$ (with A being taken constant, since the term is not needed for accuracy, only for stability).

The $\lambda^4A^4W_{4x}$ part of (15), however, is due to extending the Taylor series; i.e., it is derived from

$$
W_{4t} = (A^3F_x)_{xxx}.
\tag{17}
$$

The finite-difference representation of (17) is, to 3rd order accuracy,

$$
\begin{aligned}
[(A^3F_x)_{xxx}]^n_j = &\frac{1}{h^4}[(A^n_{j+3/2})^3(F^n_{j+2} - F^n_{j+1}) - 3(A^n_{j+1/2})^3(F^n_{j+1} - F^n_j) \\
&+ 3(A^n_{j-1/2})^3(F^n_j - F^n_{j-1}) - (A^n_{j-3/2})^3(F^n_{j-1} - F^n_{j-2})].
\end{aligned}
\tag{18}
$$

In practice, we will take the artificial viscosity term, either in its conservation form (i.e., use (16) and (18)), or in the linear version where the finite-difference form of (15) is:

$$(19)\qquad -\frac{\Omega}{24}[\lambda^2(A_j^n)^2 + \nu\lambda^4(A_j^n)^4][W_{j+2}^n - 4W_{j+1}^n + 6W_j^n - 4W_{j-1}^n + W_{j-2}^n].$$

If we examine the linear stability of the scheme in the usual von Neumann fashion, then we find that for $\Omega = \epsilon = \delta = -\nu = 1$ the criterion is $\lambda\alpha \leqq 1$ where α is the spectral radius of A. This result is also a special case of Theorem 1 in Strang's paper of 1962, [8].

In principle, it is possible to build up, in the above manner, numerical schemes of any desired accuracy. It seems that such schemes of odd orders will not be linearly stable unless an artificial viscosity term is added. The artificial viscosity term that we have added contains a term which is proportional to the next higher even derivative of the Taylor series development of $W(x, t + \Delta t)$. Thus, it might be possible to take just that amount of artificial viscosity which will not only stabilize the scheme, but also will add one more order of truncation accuracy. Of course, when doing this, care has to be taken that all the differencing is consistent with the higher order accuracy. In effect, this is the case with the Lax-Wendroff term, which might be considered as a stabilizing term added to a first order scheme. If the coefficient of $(AF_x)_x$ is cleverly chosen to be $\Delta t^2/2!$, then an additional bonus is the 2nd order accuracy.

5. Analytic Solutions for Comparison Purposes. Consider the single (scalar) equation $u_t + A(u)u_x = 0$, with the initial conditions $u(x, 0) = \Phi(x)$. This hyperbolic equation has straight characteristics whose slope is given by $dt/dx = 1/A(u)$. Since u is known at $t = 0$, and since u remains constant along a characteristic, it is easy to find analytic solutions to the above initial-value problem with $A(u) = u$ and $\Phi(x) = x^\alpha$, $\alpha = 0, 1, 2, \frac{1}{2}, \frac{1}{3}$:

$$(20)\qquad \alpha = 0: \qquad u(x, t) = 1,$$

$$(21)\qquad \alpha = 1: \qquad u(x, t) = x/(1 + t),$$

$$(22)\qquad \alpha = 2: \qquad u(x, t) = \frac{2xt + 1 - (1 + 4xt)^{1/2}}{2t^2},$$

$$(23)\qquad \alpha = \tfrac{1}{2}: \qquad u(x, t) = \frac{(t^2 + 4x - t)^{1/2}}{2},$$

$$(24)\qquad \alpha = \tfrac{1}{3}: \qquad u(x, t) = z^{1/3} - \frac{t}{3}z^{-1/3}, \quad \left(z = \frac{x}{2} + \left(\frac{x^2}{4} + \frac{t^3}{27}\right)^{1/2}\right).$$

We shall take these solutions at $x = 0$ and $x = 1$ to serve as the boundary conditions for the numerical work which is to be checked in $0 < x < 1$ against the above analytic solutions.

The case of a solution containing a discontinuity which is created at some $t = t_c$ is demonstrated by taking the following initial conditions:

$$(25)\qquad \begin{aligned} \Phi(x) &= 1, & -\infty < x \leqq \theta, \\ &= 2 - x/\theta, & \theta \leqq x \leqq 2\theta, \\ &= 0, & 2\theta \leqq x < \infty. \end{aligned}$$

The solution is given by

$$
(26)\qquad
\begin{aligned}
u(x, t) &= 1, && -\infty < x \leqq t + \theta, \\
&= \frac{2\theta - x}{\theta - t}, && t + \theta \leqq x \leqq 2\theta \quad (0 \leqq t < \theta), \\
&= 0, && 2\theta \leqq x < \infty
\end{aligned}
$$

and for $t \geqq t_c = \theta$:

$$
(27)\qquad
\left.
\begin{aligned}
u(x, t) &= 1, && -\infty < x \leqq \tfrac{1}{2}(t + 3\theta), \\
&= 0, && \tfrac{1}{2}(t + 3\theta) < x \leqq 1,
\end{aligned}
\right. \quad (t \geqq \theta).
$$

The "shock-wave" is created at time $t_c = \theta$ and at the location $x = 2\theta$, and moves to the right with the speed $\dot{x}_s = \frac{1}{2}$. In the numerical computations corresponding to this case, we shall examine the behavior of the solution also across the discontinuity and compare it to both the analytic solution and the results obtained from the standard Lax-Wendroff method.

6. Numerical Results. In reporting on the numerical work, we shall compare the standard Lax-Wendroff results with those of our third order scheme (Eq. (14)), either with the linear viscosity (Eq. (19)) or with the conservation form artificial viscosity ((16) and (18)).

6a. *An Example for Smooth Solutions.* We take $\Delta x = 0.005$, $u(x, 0) = \Phi(x) = x^2$ and, from (22),

$$
u(0, t) = 0, \qquad u(1, t) = \frac{2t + 1 - (1 + 4t)^{1/2}}{2t^2}.
$$

As expected, the maximum relative error using the scheme presented above is about 100 times smaller than the one given by the standard Lax-Wendroff method. This is the case when we use the linear artificial viscosity (Eq. (19)). When the conservation form of the artificial viscosity is used, the ratio of the maximum relative errors decreases from about 1/100 to about 1/1000.

6b. *An Example for Discontinuous Solutions.* Here, we take $u_t + uu_x = 0$ with the initial distribution (25) and boundary conditions according to (26) and (27). The results indicate that the 3rd order accuracy scheme gives a slight improvement over the L-W calculation in the large gradient region, in the sense that the "shock" is slightly steeper and the post-shock oscillations are weaker and are damped more quickly. On the other hand, unlike the L-W case, there is a very small negative perturbation ahead of the "shock". The appearance of this precursor perturbation is due to the fact that in the 3rd order scheme, in addition to u_j and $u_{j\pm1}$, one also uses $u_{j\pm2}$.

7. A Fourth Order Finite-Difference Scheme. As was mentioned before, if, in the term stemming from W_{tt}, we represent $A^n_{j\pm1/2}$ by a higher order interpolation formula, and if we take $\Omega = 1$, then our scheme becomes of fourth order accuracy. This is in line with the remarks at the end of Section 3—adding a stabilizing term to an odd order scheme can raise the order of accuracy if the coefficients of this added derivative are chosen properly.

In the present case, the fourth order finite-difference scheme has the following form:

$$
\begin{aligned}
W_i^{n+1} = {} & W_i^n + \lambda\left[\tfrac{1}{2}(F_{i+1}^n - F_{i-1}^n) - \frac{\delta}{12}(F_{i+2}^n - 2F_{i+1}^n + 2F_{i-1}^n - F_{i-2}^n)\right] \\
& + \frac{\lambda^2}{2!}\Big\{\tilde{A}_{i+1/2}^n(F_{i+1}^n - F_i^n) - \tilde{A}_{i-1/2}^n(F_i^n - F_{i-1}^n) \\
& \quad - \frac{\Omega}{12}[\tilde{A}_{i+3/2}^n(F_{i+2}^n - F_{i+1}^n) - 3\tilde{A}_{i+1/2}^n(F_{i+1}^n - F_i^n) + 3\tilde{A}_{i-1/2}^n(F_i^n - F_{i-1}^n) \\
& \quad - \tilde{A}_{i-3/2}^n(F_{i-1}^n - F_{i-2}^n)]\Big\} \\
& + \epsilon\frac{\lambda^3}{3!}\{\tfrac{1}{2}(A_{i+1}^n)^2(F_{i+2}^n - F_i^n) - (A_i^n)^2(F_{i+1}^n - F_{i-1}^n) + \tfrac{1}{2}(A_{i-1}^n)^2(F_i^n - F_{i-2}^n)\} \\
& + \Omega\frac{\lambda^4}{4!}\{(A_{i+3/2}^n)^3(F_{i+2}^n - F_{i+1}^n) - 3(A_{i+1/2}^n)^3(F_{i+1}^n - F_i^n) \\
& \quad + 3(A_{i-1/2}^n)^3(F_i^n - F_{i-1}^n) - (A_{i-3/2}^n)^3(F_{i-1}^n - F_{i-2}^n)\}
\end{aligned} \tag{28}
$$

where

$$
\tilde{A}_{i\pm1/2}^n = \tfrac{1}{2}(A_{i\pm1}^n + A_i^n) - \frac{\mu}{16}(A_{i\pm2}^n - A_{i\pm1}^n - A_i^n + A_{i\mp1}^n). \tag{29}
$$

Scheme (28) meets the stability criterion $\lambda\alpha \leqq 1$. Note that if $\mu = 0$, then Eq. (28) is the 3rd order scheme with the linear artificial viscosity represented in a conservative form. If also $\delta = \epsilon = \Omega = 0$, then we have the Lax-Wendroff scheme. For the fourth order accuracy, we must use $\delta = \epsilon = \Omega = \mu = 1$. We ran test runs with $\Phi(x) = x^\alpha$ in order to determine in practice, and compare to prediction, the amount by which the grid can be coarsened and still maintain the same maximum relative error as we go from Lax-Wendroff to 3rd order and then 4th order schemes. The grid sizes (based on $\Delta x = .005$ for the L-W scheme) were found to be, respectively: $\Delta x_{\text{L.W.}} = .1/200$; $\Delta x_{\text{3rd Order}} = .1/50$; and $\Delta x_{\text{4th Order}} = .1/25$. These grids produce absolute errors of $C \cdot 10^{-6}$ where for $\alpha = 2$ and $t \simeq 3$, $1 < C < 5$.

In conclusion, it may be stated that a 3rd or 4th order scheme, such as the schemes proposed in this paper, will, in the smooth part of the solution to a hyperbolic problem, yield, in practice as well as in theory, one or two orders of accuracy higher than, say, the Lax-Wendroff method. In the regions near shock-like discontinuities, the improvement over the L-W scheme is not as good. This opens up the possibility that in multidimensional cases, we shall be able in a practical manner to overcome partially the problems of restricted machine memory by using coarser grids and higher order schemes.

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